

Mott scattering at the interface between a metal and a topological insulator

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We compute the spin-active scattering matrix and the local spectrum at the interface between a metal and a three-dimensional topological band insulator. We show that there exists a critical incident angle at which complete (100%) spin flip reflection occurs and the spin rotation angle jumps by π . We discuss the origin of this phenomena, and systematically study the dependence of spin-flip and spin-conserving scattering amplitudes on the interface transparency and metal Fermi surface parameters. The interface spectrum contains a well-defined Dirac cone in the tunneling limit, and smoothly evolves into a continuum of metal induced gap states for good contacts. We also investigate the complex band structure of Bi_2Se_3 .

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I. INTRODUCTION

Recently discovered three dimensional topological band insulators¹⁻³, such as $\text{Bi}_{1-x}\text{Sb}_x$ ⁴ and Bi_2Se_3 ⁵⁻⁷, are spin-orbit coupled crystal solids with a bulk gap but protected gapless surface states. The low energy excitations at the surface are helical Dirac fermions, i.e., their spin and momentum are entangled (locked)⁸. The charge and spin transport on the surface of a topological insulator are intrinsically coupled⁹. This makes these materials a promising new platform for spintronics. In addition, heterostructures involving topological insulator, superconductor, and/or ferromagnet have been predicted to show a remarkable array of novel spectral and transport properties (for review see Ref.¹⁰⁻¹²).

Electronic or spintronic devices based on topological insulators will almost inevitably involve metal as measurement probes or functioning components¹³. This motivates us to study the local spectrum near the interface between a metal (M) and a topological insulator (TI). For a metal-ordinary semiconductor junction with good contact, it is well known that the metallic Bloch states penetrate into the semiconductor as evanescent waves localized at the interface (for energies within the band gap). Such interface states are known as metal induced gap states (MIGS)^{14,15}. They play an important role in controlling the junction properties, e.g., by pinning the semiconductor Fermi level to determine the Schottky barrier height¹⁶, a key parameter of the junction.

The local spectrum at the M-TI junction is intimately related to the spin-active scattering of electrons at the M-TI interface. In this paper, we systematically study the evolution of the scattering matrix and the interface spectra with the junction transparency and metal Fermi surface parameters. The scattering matrix¹⁷ we obtain here also forms the basis to investigate the details of the superconducting proximity effect near the superconductor-TI interface¹⁸, which was shown by Fu and Kane to host Majorana fermions¹⁹.

The scattering at the M-TI interface differs signifi-

cantly from its two dimensional analog, the interface between a metal and a quantum spin Hall (QSH) insulator studied by Tokoyama et al¹³. They predicted a giant spin rotation angle $\alpha \sim \pi$ and interpreted the enhancement as resonance with the one-dimensional helical edge modes. By contrast, for M-TI interface we predict a critical incident angle at which complete spin flipping occurs and the spin rotation angle jumps by π . We will explain its origin, in particular its relation to the surface helical Dirac spectrum, and discuss its spintronic implications.

This paper is organized as follows. We will first compute the scattering matrix using a $\mathbf{k} \cdot \mathbf{p}$ continuum model by matching the envelope wave functions at the M-TI interface. This simple calculation is easy to understand, and it brings out the main physics of our problem. Along the way, we will discuss the complex band structure of Bi_2Se_3 , which describes the decaying (rather than propagating Bloch wave) solutions of the crystal Hamiltonian. The various caveats of this calculation are then remedied by considering a much more general lattice model. Most importantly, it enables us to track how the scattering matrix and interface spectrum change with interface transparency. It also sheds light on the origin of perfect spin-flip scattering at the critical angle. We will show that the results obtained from these two complementary methods are consistent with each.

II. MODEL HAMILTONIAN AND COMPLEX BAND STRUCTURE

We consider Bi_2Se_3 as a prime example of 3D strong topological insulators. Its low energy $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian was obtained by Zhang et al⁶,

$$\hat{H}_{TI}(\mathbf{k}) = \epsilon_0(\mathbf{k})\hat{1} + \sum_{\mu=0}^3 d_{\mu}(\mathbf{k})\hat{\Gamma}_{\mu}.$$

Here $d_0(\mathbf{k}) = M - B_1k_z^2 - B_2(k_x^2 + k_y^2)$, $d_1(\mathbf{k}) = A_2k_x$, $d_2(\mathbf{k}) = A_2k_y$, $d_3(\mathbf{k}) = A_1k_z$, and $\epsilon_0(\mathbf{k}) = C + D_1k_z^2 +$

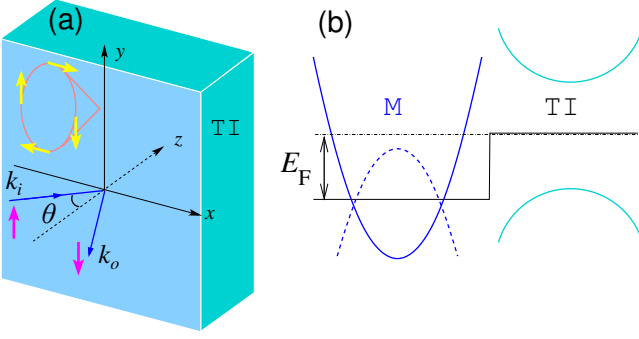


FIG. 1: (a) Scattering geometry at a metal (M)-topological insulator (TI) interface. (b) Schematic band structure of the metal (modeled by \hat{H}_M) and topological insulator.

$D_2(k_x^2 + k_y^2)$. The numerical values of M, A, B, C, D are given in Ref.⁶. We choose the basis ($|+\uparrow\rangle, |+\downarrow\rangle, |-\uparrow\rangle, |-\downarrow\rangle$), where \pm labels the hybridized p_z orbital with even (odd) parity⁶. The Gamma matrices are defined as $\hat{\Gamma}_0 = \hat{\tau}_3 \otimes \hat{1}$, $\hat{\Gamma}_i = \hat{\tau}_1 \otimes \hat{\sigma}_i$, with $\hat{\tau}_i$ ($\hat{\sigma}_i$) being the Pauli matrices in the orbital (spin) space. The chemical potential of as-grown Bi_2Se_3 crystal actually lies in the conduction band⁸. By hole doping⁸ or applying a gate voltage²⁰, the chemical potential can be tuned inside the gap. The system is well described by H_{TI} (note that energy zero is set as in the middle of the band gap).

In this section, we first adopt a rather artificial model for metals with negligible spin-orbit coupling. It is obtained by turning off the spin-orbit interaction (setting $d_\mu = 0$ for $\mu=1,2,3$) in H_{TI} and shifting the Fermi level into the conduction band. The result is spin-degenerate two-band Hamiltonian

$$\hat{H}_M(\mathbf{k}) = [\epsilon_0(\mathbf{k}) - E_F]\hat{1} + d_0(\mathbf{k})\hat{\Gamma}_0.$$

Its band structure, schematically shown in Fig. 1(b), consists of two oppositely dispersing bands (the solid and dash line). E_F is tuned to be much higher than the band crossing point, so the scattering properties of low energy electrons near the Fermi surface are insensitive to the band crossing at high energies. This claim will be verified later using a more generic model for the metal. A similar model was used in the study of metal-QSH interface¹³.

Matching the wave functions of two dissimilar materials (such as Au and Bi_2Se_3) at interface is in general complicated within the $\mathbf{k} \cdot \mathbf{p}$ formalism, because the envelope wave functions on either side are defined using different basis (see Ref. 21 and reference therein). For the particular model H_M , however, such complication is circumvented. Then, the wave functions at the metal-TI interface ($z = 0$) satisfy the Ben-Daniel and Duke boundary condition²²,

$$\hat{\Phi}_M = \hat{\Phi}_{TI}, \quad \hat{v}_M \hat{\Phi}_M = \hat{v}_{TI} \hat{\Phi}_{TI}.$$

Here $\hat{\Phi}_i$ is the four-component wave function, and the velocity matrix $\hat{v}_i = \partial \hat{H}_i / \partial k_z$, $i \in \{M, TI\}$. Such bound-

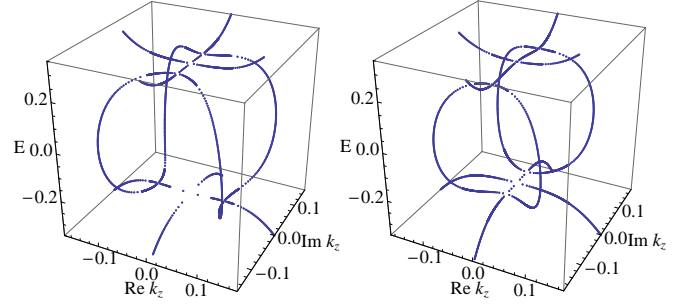


FIG. 2: The complex band structure of topological insulator described by $\hat{H}_{TI}(\mathbf{k})$ for $k_y = 0$, $k_x = 0.02$ (left) and 0.04 (right). E is measured in eV, and k in \AA^{-1} . Subgap states with complex k_z represent evanescent waves. The topology of real lines²⁵ changes as k_x is increased.

ary condition assumes good atomic contact between two materials.

We are interested in energies below the band gap of TI, so $\hat{\Phi}_{TI}$ is evanescent in nature and only penetrates into TI for a finite length. Such localized (surface or interface) states inside topological insulator can be treated within the $\mathbf{k} \cdot \mathbf{p}$ formalism using the theory of *complex band structures*, pioneered by Kohn²³, Blount²⁴, and Heine²⁵ et al. The main idea is to allow the crystal momentum to be complex and analytically continue $H_{TI}(\mathbf{k})$ to the complex \mathbf{k} plane. While the extended Bloch waves are the eigen states of $H_{TI}(\mathbf{k})$ for real \mathbf{k} , eigen functions of $H_{TI}(\mathbf{k})$ for complex \mathbf{k} describe localized states. Together they form a complete basis to describe crystals of finite dimension.

In our scattering problem, we have to find all eigen states of $H_{TI}(\mathbf{k})$ with energy E and wave vector $\mathbf{k} = (k_x, k_y, \tilde{k}_z)$, where k_x and k_y are given and real, but \tilde{k}_z is complex and unknown. For a general $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian such as \hat{H}_{TI} , we follow Chang and Schulman²⁶ to rewrite it as

$$\hat{H}_{TI} = \hat{h}_0(k_x, k_y) + \hat{h}_1 \tilde{k}_z + \hat{h}_2 \tilde{k}_z^2,$$

where $\hat{h}_1 = A_1 \hat{\Gamma}_3$, and $\hat{h}_2 = -B_1 \hat{\Gamma}_0$. Then the eigen equation $(\hat{H}_{TI} - E\hat{1})\hat{\phi} = 0$ can be reorganized into an eigen value problem for \tilde{k}_z ,

$$\begin{pmatrix} 0 & 1 \\ -\hat{h}_2^{-1}(\hat{h}_0 - E\hat{1}) & -\hat{h}_2^{-1}\hat{h}_1 \end{pmatrix} \begin{pmatrix} \hat{\phi} \\ \hat{\phi}' \end{pmatrix} = \tilde{k}_z \begin{pmatrix} \hat{\phi} \\ \hat{\phi}' \end{pmatrix}.$$

Then all possible values of \tilde{k}_z can be obtained for given incident parameter E, k_x , and k_y . For the anisotropic Dirac Hamiltonian $H_{TI}(\mathbf{k})$, the energy eigenvalues can be obtained analytically²⁸, which allows for an analytical solution of the complex band structure.

For E within the gap, there are in general 4 pairs of complex solution of k_z , for if \tilde{k}_z is a solution so is \tilde{k}_z^* . We label those with positive imaginary parts with $\{\tilde{k}_z^\nu\}$, and the corresponding wave function $\{\hat{\phi}^\nu\}$, $\nu = 1, 2, 3, 4$. They are decaying solutions in the half space $z > 0$.

In our model, \tilde{k}_z turns out to be doubly degenerate, as shown in Fig. 2. The wave function inside TI ($z > 0$) then has the form

$$\hat{\Phi}_{TI} = \sum_{\nu} t_{\nu} e^{i\tilde{k}_z^{\nu} z} \hat{\phi}_{\nu}.$$

III. SCATTERING MATRIX FROM WAVE-FUNCTION MATCHING

To set the stage for discussing scattering off a topological insulator, it is instructive to recall the generic features of elastic scattering of electrons by a heavy ion with spin-orbit interaction. This classical problem was solved by Mott, and known as *Mott scattering*. The scattering matrix has the general form²⁷

$$\hat{S}_{Mott} = u\hat{1} + w\hat{\sigma} \cdot (\mathbf{k}_i \times \mathbf{k}_o),$$

where \mathbf{k}_i and \mathbf{k}_o are the incident and outgoing momentum respectively, $\hat{\sigma}$ is the Pauli matrix, and u, w depend on the scattering angle. It is customary to define the spin-flip amplitude $f = S_{21}$, and spin-conserving amplitude $g = S_{11}$. Both f and g are complex numbers, their relative phase defines the *spin rotation angle* $\alpha = \text{Arg}(g^* f)$. One immediately sees that for back scattering, $\hat{S}_{Mott} = u\hat{1}$, so there is no spin flip, $f = 0$. As we will show below, this also holds true for scattering off TI.

Now consider an electron coming from the metal with momentum \mathbf{k} incident on the M-TI interface located at $z = 0$, as schematically shown in Fig. 1(a). We assume the interface is translationally invariant, so the transverse momentum $\mathbf{k}_{\parallel} = (k_x, k_y)$ is conserved, and the energy E of the electron lies within the band gap of TI. Then, only total reflection is possible, but the spin-orbit coupling inside TI acting like a \mathbf{k} -dependent magnetic field rotates the spin of the incident particle. The scattering (reflection) matrix has the form

$$\hat{S}(\mathbf{k}) = \begin{pmatrix} g & \bar{f} \\ f & \bar{g} \end{pmatrix},$$

where $|g|^2 + |f|^2 = 1$. Our goal is to find the dependence of the scattering amplitudes f, g on \mathbf{k} , or equivalently, on energy E and incident angle θ . From time-reversal symmetry, $\bar{f}(E, \theta) = f(E, -\theta)$ and $\bar{g}(E, \theta) = g(E, -\theta)$. We shall show that $f(\mathbf{k}_{\parallel}) = -f(-\mathbf{k}_{\parallel})$, $g(\mathbf{k}_{\parallel}) = g(-\mathbf{k}_{\parallel})$. So f is an odd function of θ , while g is even in θ . Since our problem can be viewed as coherent multiple scattering from a lattice array of Mott scatters occupying half the space, we will refer to spin-active scattering at the metal-TI interface as Mott scattering.

Consider a spin up electron from the conduction band of the metal with momentum \mathbf{k} and energy $E = \epsilon_0(\mathbf{k}) - E_F - d_0(\mathbf{k})$ lying within the band gap of TI. The wave function inside the metal ($z < 0$) has the form

$$\hat{\Phi}_M = (r_1 e^{-ik'_z z}, r_2 e^{-ik'_z z}, e^{ik_z z} + r_3 e^{-ik_z z}, r_4 e^{-ik_z z})^T,$$

up to the trivial $e^{i(k_x x + k_y y)}$ and renormalization factor. Here $k_z = \hat{z} \cdot \mathbf{k}$, and $\{r_i\}$ are the reflection amplitudes. We identify the spin flip amplitude $f = r_4$ and the spin-conserving amplitude $g = r_3$. Note that there is no propagating mode at energy E available in the valence band for the reflected electron. So k'_z is purely imaginary. At such energy, there is no propagating mode available in TI. We have discussed the evanescent wave function $\hat{\Phi}_{TI}$ in the previous section. With $\hat{\Phi}_M$ and $\hat{\Phi}_{TI}$, we solve the boundary condition at $z = 0$ to obtain r_{ν}, t_{ν} and the scattering matrix S .

Fig. 3 shows the magnitude and phase of f and g versus the incident angle θ for $E = 0.1\text{eV}$, with E_F set to be 0.28eV . At normal incidence, $\theta = 0$, spin flip scattering is forbidden as in the single-ion Mott scattering. With increasing θ the magnitude of g drops continuously. At a critical angle θ_c , $|g|$ drops to zero and we have perfect (100%) spin flip reflection. At the same time, the spin rotation angle α (the relative phase between f and g) jumps by π .

It is tantalizing to think of what happens at θ_c as resonant scattering with the helical surface mode of the TI. This however is problematic. We are considering good contacts at which the wave functions of the two materials hybridize strongly. Surface mode is preempted by MIGS. Indeed, we checked that the corresponding critical transverse momentum k_{\parallel} depends only weakly on E . This is at odds with the linear dispersion of the TI surface mode, $E = A_2 k_{\parallel}$ ⁶. To gain better understanding, we now switch to a lattice model to systematically study the role of interface transparency and metal Fermi surface parameter (E_f, k_f, v_f) on the scattering matrix.

IV. INTERFACE SPECTRUM AND SCATTERING MATRIX FROM LATTICE GREEN FUNCTION

We consider a simple lattice model for the M-TI junction. The topological insulator is modeled by a tight binding Hamiltonian on cubic lattice,

$$\mathcal{H}_R = \sum_{\mathbf{k}_{\parallel}, n} \left\{ \hat{\psi}_{\mathbf{k}_{\parallel}, n}^{\dagger} (b_1 \hat{\Gamma}_0 - i \frac{a_1}{2} \hat{\Gamma}_3) \hat{\psi}_{\mathbf{k}_{\parallel}, n+1} + h.c. + \hat{\psi}_{\mathbf{k}_{\parallel}, n}^{\dagger} \left[d(\mathbf{k}_{\parallel}) \hat{\Gamma}_0 + a_2 (\hat{\Gamma}_1 \sin k_x + \hat{\Gamma}_2 \sin k_y) \right] \hat{\psi}_{\mathbf{k}_{\parallel}, n} \right\}.$$

Here $\hat{\psi} = (\psi_{+\uparrow}, \psi_{+\downarrow}, \psi_{-\uparrow}, \psi_{-\downarrow})^T$ is the annihilation operator, $d(\mathbf{k}_{\parallel}) = M - 2b_1 + 2b_2(\cos k_x + \cos k_y - 2)$ with k measured in $1/a$. The cubic lattice consists of layers of square lattice stacked in the z direction, n is the layer index, and \mathbf{k}_{\parallel} is the momentum in the xy plane. The isotropic version of \mathcal{H}_R , with $a_1 = a_2$, $b_1 = b_2$, was studied by Qi et al as a minimal model for 3D topological insulators²⁸. To mimic Bi_2Se_3 , we set the lattice spacing $a = 5.2\text{\AA}$, which gives the correct unit cell volume, and $a_i = A_i/a$, $b_i = B_i/a^2$ for $i = 1, 2$. Although a crude caricature of the real material, \mathcal{H}_R yields the correct gap

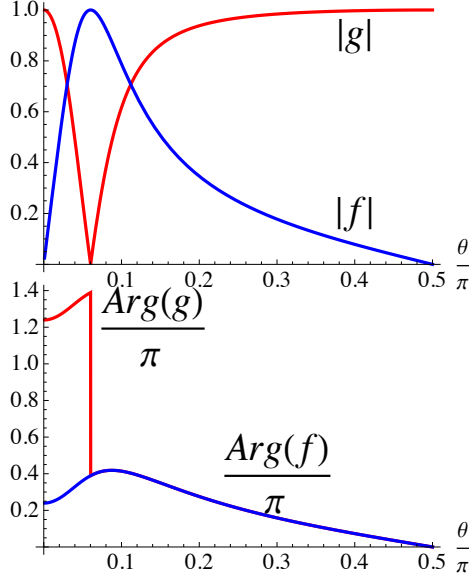


FIG. 3: The magnitudes (upper panel) and the phases (lower panel) of the spin-flip amplitude f and spin-conserving amplitude g versus the incident angle θ . $E = 0.1\text{eV}$, $E_F = 0.28\text{eV}$. $|g|^2 + |f|^2 = 1$. $\text{Arg}(g)$ and $\text{Arg}(f)$ are shifted upward by π for clarity.

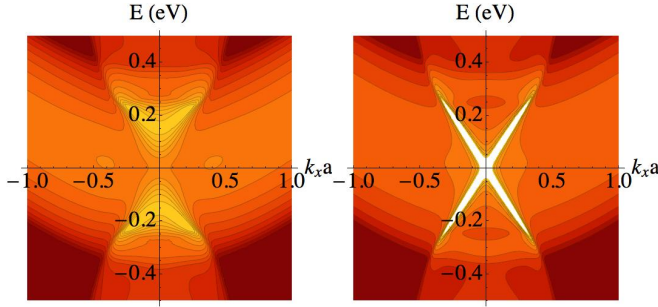


FIG. 4: The spectral function $N(E, k_x, k_y = 0)$ at the interface of metal and topological insulator. Left: good contact, $J = t_M$, showing the continuum of metal induced gap states. Right: poor contact with low transparency, $J = 0.2t_M$, showing well defined Dirac spectrum as on the TI surface. $t_M = 0.18\text{eV}$, $\mu_M = -4t_M$, a is lattice spacing.

size and surface dispersion, it also reduces to the continuum $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian \hat{H}_{TI} in the small k limit, aside from the topologically trivial $\epsilon_0(\mathbf{k})$ term.

As a generic model for metal, we consider a single band tight binding Hamiltonian on cubic lattice,

$$\mathcal{H}_L = \sum_{\mathbf{k}_{\parallel}, n, \sigma} [h(\mathbf{k}_{\parallel})n_{\mathbf{k}_{\parallel}, n, \sigma} - t_M \phi_{\mathbf{k}_{\parallel}, n, \sigma}^{\dagger} \phi_{\mathbf{k}_{\parallel}, n+1, \sigma} + h.c.]$$

where $h(\mathbf{k}_{\parallel}) = -2t_M(\cos k_x + \cos k_y) - \mu_M$. The Fermi surface parameters of the metal can be varied by tuning t_M and μ_M . The metal occupies the left half space, $n \leq 0$, and the TI occupies the right half space $n \geq 1$. The interface domain consists of layer $n = 0, 1$. The coupling

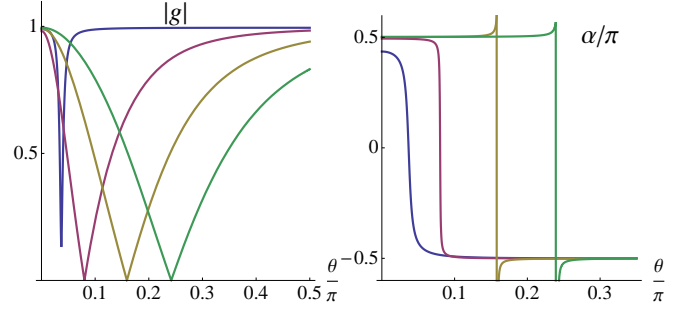


FIG. 5: The spin-conserving reflection amplitude $|g|$ and spin rotation angle α versus the incident angle θ for increasing contact transparency, $J/t_M = 0.25, 1, 1.5, 2$ (from left to right). $t_M = 0.18\text{eV}$, $\mu_M = -4t_M$, $E = 0.05\text{eV}$, $k_y = 0$. $|f|^2 = 1 - |g|^2$.

between metal and TI is described by hopping,

$$\mathcal{H}_{LR} = - \sum_{\mathbf{k}_{\parallel}, \ell, \sigma} J_{\ell} \psi_{\mathbf{k}_{\parallel}, n=1, \ell, \sigma}^{\dagger} \phi_{\mathbf{k}_{\parallel}, n=0, \sigma} + h.c.$$

J_{ℓ} is the overlap integral between the p -orbital $\ell = \pm$ of TI and the s -like orbital of metal. For simplicity, we assume J_{ℓ} is independent of spin. Then, $J_+ = -J_- = J$. J can be tuned from weak to strong. Small J mimics a large tunneling barrier between M and TI, and large J (comparable to t_M or B_2) describes a good contact.

The lattice Green function of the composite system is computed via standard procedure by introducing the inter-layer transfer matrix and the method of interface Green function matching²⁹. Fig. 4 shows two examples of the local spectral function (momentum-resolved density of states) at the interface,

$$N(E, \mathbf{k}_{\parallel}) = - \sum_{n=0,1} \text{ImTr} \hat{\mathcal{G}}(E, \mathbf{k}_{\parallel})_{n,n},$$

where $\hat{\mathcal{G}}(E, \mathbf{k}_{\parallel})_{n,n'}$ is the local Green function at the interface with $n, n' = 0, 1$, and the trace is over the spin and orbital space. In the tunneling (weak coupling, small J) limit, the interface spectrum includes a sharply defined Dirac cone as on the surface of TI. As J is increased, the linearly dispersing mode becomes ill defined and eventually replaced by a continuum of metal induced gap states.

Once the lattice Green function is known for given incident E and k_{\parallel} , the scattering (reflection) matrix can be constructed from $\hat{\mathcal{G}}$ by²⁹,

$$\hat{S}(E, \mathbf{k}_{\parallel}) = \hat{\mathcal{G}}(E, \mathbf{k}_{\parallel})_{0,0} g_M^{-1}(E, \mathbf{k}_{\parallel}) - \hat{1}$$

where g_M is the spin-degenerate bulk Green function of metal. Fig. 5 shows the evolution of $|g(\theta)|$ and $\alpha(\theta)$ for increasing J , where a level broadening of $E/10$ is used. Most importantly, we observe that the existence of a critical angle θ_c , where complete spin-flip occurs and α jumps by π , is a robust phenomenon. It is independent of the details of the contact, the metal Fermi surface, or other high energy features in the band structure.

To understand the perfect spin flip, we first focus on the tunneling limit, $J \ll t_M$. In this limit, the local spectrum at layer $n = 1$ as shown in the right panel of Fig. 4 approaches the TI surface spectrum, namely the helical Dirac cone. An incident up spin tunneling across the barrier will develop resonance with the helical mode, which is a quasi-stationary state with long life time, if its momentum and energy satisfy $k_{\parallel} = E/A_2$. Moreover, it has to flip its spin, since only down spin can propagate in the k_x direction (suppose $k_y = 0$). The π jump in the phase shift is also characteristic of the resonance. Indeed, we have checked that precisely at θ_c the resonance criterion, $k_f \sin \theta_c = E/A_2$, is met. We also varied μ_M for fixed J and t_M , bigger μ_M yields a bigger Fermi surface and a smaller θ_c . This is consistent with the resonance criterion above.

As J is increased, the width of the resonance grows and eventually it is replaced by a broad peak (dip) in $|f|$ ($|g|$), but the vanishing of $|g|$ and π shift in α at θ_c persist to good contacts, even though in this limit the interface is flooded by MIGS (left panel of Fig. 4) and bears little resemblance to the Dirac spectrum. With all other parameters held fixed, θ_c increases with J . Qualitatively, coupling to TI renormalizes the metal spectrum near the interface, producing a smaller effective k_f (hence a larger θ_c) compared to its bulk value. It is remarkable that perfect spin flip at the critical angle persists all the way from poor to good contacts. Indeed, the main features observed here for good contacts using the lattice model agree well with the results obtained in previous section by wave function matching.

V. DISCUSSIONS

We now discuss the experimental implications of our results. The M-TI interface spectrum can be measured

by ARPES (or scanning tunneling microscope) experiments on metal film coated on a topological insulator. Our results also suggest that a topological insulator can serve as a perfect mirror to flip the electron spin in metal. Such spin-active scattering at the M-TI interface may be exploited to make novel spintronic devices. The magnitude of g or f can be measured by attaching two ferromagnetic leads to a piece of metal in contact with TI, forming a multi-terminal device. One of the ferromagnetic leads produces spin-polarized electrons incident on the M-TI interface at some angle, while the other lead detects the polarization of reflected electron, as in a giant magneto-resistance junction. The spin rotation angle α can be measured indirectly by comparing the predicted current-voltage characteristics of M-TI-M or Superconducto-TI-Superconductor junctions, which are sensitive the phase shift α . It can also be inferred from the spin transport in a TI-M-TI sandwich, as discussed for QSH insulator in Ref.¹³. Detailed calculations of the transport properties of these structured, using the scattering matrix obtained here, will be subjects of future work.

VI. ACKNOWLEDGEMENTS

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